

Cyclosarin
329-99-7 | DTXSID00861875

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 91.3 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.10e-01

Confidence level: 7.73e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Acetamide, N-(4-bromophenyl)-

Measured: 89.1

Predicted: 93.9

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3,4-Dichloroacetanilide

Measured: 219

Predicted: 111

[Image not found](#)

Acetamide, N-(3-chlorophenyl)-

Measured: 72.4

Predicted: 55.5

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Acetamide, N-(2-chlorophenyl)-

Measured: 38.0

Predicted: 49.2

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Acetamide, N-(3-bromophenyl)-
(9CI)

Measured: 102

Predicted: 77.2